Momentum Dependence of π-π* Excitations of Benzene Rings in Condensed Phases

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Abstract No. Haya1243
Beamline(s): **X21**

Introduction: The measurements of the real (ε_1) and the imaginary (ε_2) parts of the dielectric function (DF) over a complete momentum (q) - energy (E) range provide a crucial basis for studies of radiation in matter. Unfortunately, knowledge of the DF for molecular liquids is quite insufficient, especially for q ~ 1, because of the lack of appropriate experimental tools. With the developments of synchrotron radiation sources, however, it is now possible to apply inelastic x-ray scattering (IXS) to determine the DF of molecular liquids for q <~ 1.

Methods and Materials: IXS spectra for the π–π* excitation of liquid benzene have been measured for 0.35<q<1.5Å^{-1} at the X21, with 0.5eV-resolution for E<10eV to resolve the π–π* peak and 1.3eV-resolution for E>10eV to achieve high S/N ratio.

Results: The ε_1 and the ε_2 of benzene were deduced from the IXS spectra via the Kramers-Kronig transformation, and were shown in Fig. 1. Although the π–π* peak in the IXS profiles shows a negative q-dispersion (~0.5eV), no marked peak dispersion is found for the ε_2, indicating that the π–π* excitation in liquid is well localized. On the other hand, the amplitude of the variation in the ε_1 is reduced significantly as q increases. Thus the negative dispersion in the IXS spectra must be attributed to changes of the shielding factor, $\varepsilon_1^2+\varepsilon_2^2$. This result means that the experimental deduction of not only energy-loss spectra but also DF on target molecular condensates is indispensable.

Acknowledgments: H.H. thanks the JSPS for the Postdoctoral Fellowships for Research Abroad (1998).

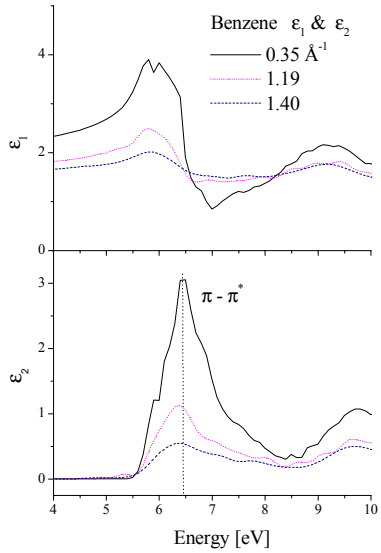

Figure 1. The ε_1 and the ε_2 of liquid benzene.